10/857,465

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NEWS 4	AUG 02	IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
NEWS 5	AUG 02	CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
NEWS 6	AUG 02	The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
NEWS 7	AUG 27	BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 8	AUG 27	BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC
NEWS 9	SEP 01	INPADOC: New family current-awareness alert (SDI) available
NEWS 10	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS 11	SEP 01	New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS 12	SEP 27	STANDARDS will no longer be available on STN
NEWS 13	SEP 27	SWETSCAN will no longer be available on STN

NEWS EXPRESS	JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 18:16:29 ON 26 OCT 2004

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 18:16:37 ON 26 OCT 2004
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STRUCTURE FILE UPDATES: 25 OCT 2004 HIGHEST RN 769101-30-6
DICTIONARY FILE UPDATES: 25 OCT 2004 HIGHEST RN 769101-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more
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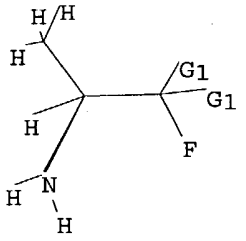
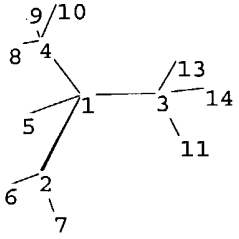
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\09857465.str





chain nodes :
1 2 3 4 5 6 7 8 9 10 11 13 14
chain bonds :
1-2 1-3 1-4 1-5 2-6 2-7 3-11 3-13 3-14 4-8 4-9 4-10
exact/norm bonds :
1-2 3-13 3-14
exact bonds :
1-3 1-4 1-5 2-6 2-7 3-11 4-8 4-9 4-10

G1:H,Cl,Br,I

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 13:CLASS 14:CLASS

Stereo Bonds:

2-1 (Single Wedge).

Stereo Chiral Centers:

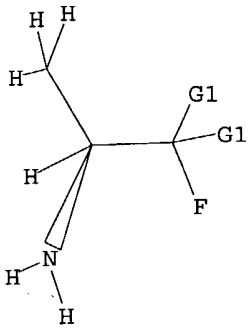
1 (Parity=Don't Care)

Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 1

L1 STRUCTURE UPLOADED

=> d query
L1 STR



G1 H,Cl,Br,I

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 18:17:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1440 TO ITERATE

69.4% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 26524 TO 31076
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 18:17:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 28548 TO ITERATE

100.0% PROCESSED 28548 ITERATIONS 17 ANSWERS
SEARCH TIME: 00.00.01

L3 17 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.42	155.63

FILE 'CAPLUS' ENTERED AT 18:17:08 ON 26 OCT 2004

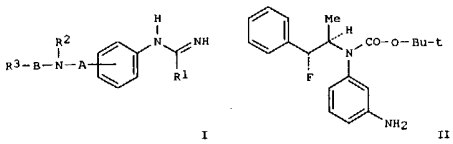
FILE COVERS 1907 - 26 Oct 2004 VOL 141 ISS 18
FILE LAST UPDATED: 25 Oct 2004 (20041025/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 13 L3

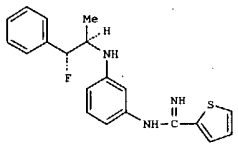
=> d l4 1-13 abs ibib hitstr

L4 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I

II



III

AB Title compds. I [R1 = (un)substituted Ph, 5-6 membered heteroaryl containing 1-3 O, S or N, atoms; R2 = H, alkyl, COO-alkyl, etc.; R3 = H, halo, (un)substituted Ph, etc.; A = CH2, CH2CH2, CH(CH3); B = halo substituted alkylene] and their pharmaceutically acceptable salts were prepared For example, coupling of aniline II, e.g., prepared from (+)-norephedrine in 6-steps, and 2-thiophenecarboximidothioic acid Me ester, followed by BOC deprotection afforded phenylthiophenecarboximidamide III dihydrochloride. Compds. I are claimed useful for the treatment of illness caused by nitric oxide synthase (no data provided).

ACCESSION NUMBER: 2003:487133 CAPLUS
DOCUMENT NUMBER: 139:52873
TITLE: Preparation of N-phenyl-2-thiophenecarboximidamides as nitric oxide synthase inhibitors
INVENTOR(S): Rehwinkel, Hartmut; Hoelscher, Peter; Jaroch, Stefan; Suelzle, Detlev; Hillmann, Margrit; Burton, Gerardine Anne; McDonald, Fiona MacDougall
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10162114	A1	20030626	DE 2001-10162114	20011212
WO 2003053914	A1	20030703	WO 2002-EP14010	20021210
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1453794	A1	20040908	EP 2002-792956	20021210
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				

PRIORITY APPLN. INFO.: DE 2001-10162114 A 20011212
WO 2002-EP14010 W 20021210

OTHER SOURCE(S): MARPAT 139:52873

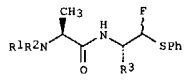
IT **370857-10-6P**, (1R,2R)-1-Fluoro-1-phenylpropan-2-amine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of phenylthiophenecarboximidamides as nitric oxide synthase inhibitors)

RN 370857-10-6 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, (αR,βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I

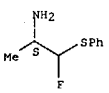
AB Fluoropeptidomimetics I (R1 = R3 = H, R2 = Boc; R1 = R3 = H, R2 = CO2Me; R1R2 = N-phthaloyl, R3 = H; R1-3 = H; R1 = H, R2 = CO2Me, R3 = Me; R1 = H, R2 = CO2Me, R3 = CH2Ph; R1 = H, R2 = CO2Me, R3 = CHMe2) and α-fluoroglycine derivative, PhCH2NHCH(F)CO2Et, were prepared as potential protease inhibitors. The stability of I was investigated under organic as well as aqueous conditions. The stability of I under acidic and basic conditions, the effect of substitution at C-2 position, and potential biol. activities were discussed.

ACCESSION NUMBER: 2003:24859 CAPLUS
DOCUMENT NUMBER: 138:221830
TITLE: Design and Synthesis of Novel Fluoropeptidomimetics as Potential Mimics of the Transition State during Peptide Hydrolysis
AUTHOR(S): Annedi, Subhash C.; Li, Weiyong; Samson, Sheeba; Kotra, Lakshmi P.
CORPORATE SOURCE: Faculty of Pharmacy, Molecular Design and Information Technology Center, and Department of Chemistry, University of Toronto, Toronto, ON, M5S 2S2, Can.
SOURCE: Journal of Organic Chemistry (2003), 68(3), 1043-1049
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:221830

IT **501121-62-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluoroglycine and fluoropeptidomimetics as potential protease inhibitors)

RN 501121-62-6 CAPLUS
CN 2-Propanamine, 1-fluoro-1-(phenylthio)-, (2S)- (9CI) (CA INDEX NAME)

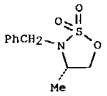
Absolute stereochemistry.

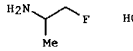


REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
GI


I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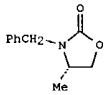
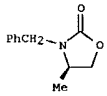

III

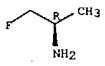

IV

AB N-benzyl [1,2,3]-oxathiazolidine 2,2-dioxides, e.g. I, (cyclic sulfamidates) were synthesized from their corresponding β-amino alcs. and used as substrates in fluorination reactions with tetrabutylammonium fluoride (TBAF). After desulfonation of the intermediates, the N-benzyl fluoroamines were debenzylated by transfer hydrogenolysis with Pd/C to yield (S) and (R)-2-amino-1-fluoropropane hydrochloride salts (II, both with 95% ee). The reactions were carried out on multi-gram scale without the need for chromatog. purification of the intermediates. In the presence of carbonate, the (S)- and (R)-N-benzylfluoroamines underwent intramol. cyclizations in which fluoride was displaced to yield cyclic carbamates III and IV.

ACCESSION NUMBER: 2002:370219 CAPLUS
DOCUMENT NUMBER: 137:232363
TITLE: Fluoroamines via chiral cyclic sulfamidates
AUTHOR(S): Posakony, Jeffrey J.; Tewson, Timothy J.
CORPORATE SOURCE: Department of Radiology Imaging Research Laboratory, University of Washington, Seattle, WA, 98195, USA
SOURCE: Synthesis (2002), (6), 766-770
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:232363
IT **273734-17-1P 458560-63-9P 459167-94-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluoroamines via chiral cyclic sulfamidates)
RN 273734-17-1 CAPLUS
CN 2-Propanamine, 1-fluoro-, hydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

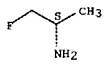
L4 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● HCl

RN 458560-63-9 CAPLUS
CN 2-Propanamine, 1-fluoro-, hydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



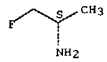
● HCl

RN 459167-94-3 CAPLUS
CN Formic acid, compd. with (2S)-1-fluoro-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 459167-93-2
CMF C3 H8 F N

Absolute stereochemistry. Rotation (+).



CM 2

CRN 64-18-6
CMF C H2 O2

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AB R1ZNHR4 [R1 = (CHR9)nNR7Z1NHR or (CHR9)nNRR7; R = NHR7- or aryl-substituted haloalkyl; R4 = H or acyl; R7 = H, (phenyl)alkyl, alkanoyl, alkoxycarbonyl; R9 = H or alkyl; Z = (un)substituted 2H-1,4-benzoxazine- or -thiazine-m,3-diyl; Z1 = alk(en)ylene; m = 5-8; n = 0-6] were prepared as neuronal nitric oxide synthase inhibitors (no data). Thus, (R)-6-aminomethyl-2-methyl-3-oxo-2H-1,4-benzoxazine was condensed with CF3CF2CHO and the product converted in 3 steps to (R)-3-amino-2-methyl-6-[(pentafluoropropylamino)methyl]-2H-1,4-benzoxazine.

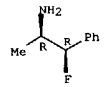
ACCESSION NUMBER: 2001:798205 CAPLUS
DOCUMENT NUMBER: 135:344492
TITLE: Preparation of benzoxazine-3-amines as neuronal nitric oxide synthase inhibitors
INVENTOR(S): Rehwinkel, Hartmut; Hoelscher, Peter; Jaroch, Stefan; Suelzle, Detlev; Hillmann, Margrit; Burton, Gerardine Anne; McDonald, Fiona McDougall
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001081323	A1	20011101	WO 2001-EP4281	20010412
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 10020667	A1	20011122	DE 2000-10020667	20000419
EP 1282610	A1	20030212	EP 2001-929561	20010412
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003531198	T2	20031021	JP 2001-578416	20010412
NO 2002005031	A	20021219	NO 2002-5031	20021018
US 2004006075	A1	20040108	US 2003-258016	20030723
PRIORITY APPLN. INFO.:			DE 2000-10020667 A	20000419
			WO 2001-EP4281 W	20010412

OTHER SOURCE(S): MARPAT 135:344492
IT **370857-10-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzoxazine-3-amines as neuronal nitric oxide synthase inhibitors)
RN 370857-10-6 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, (αR,βR)- (9CI) (CA INDEX NAME)

L4 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AB Analogs of arachidonylethanolamide (anandamide) are provided which have higher affinities for the cannabinoid CB1 and/or CB2 receptor sites. Further, most of the analogs exhibit greater metabolic stability than arachidonylethanolamide. The improved receptor affinity and selectivity and/or greater metabolic stability make these analogs therapeutically useful as medications for relief of pain caused by cancer and nausea caused by chemotherapy, as well as for peripheral pain. The compds. may also be useful as oral and topical contraceptives, in suppression of the immune system, enhancement of appetite and in treatment of psychomotor disorders, multiple sclerosis and hypertension.

ACCESSION NUMBER: 2000:383939 CAPLUS
DOCUMENT NUMBER: 133:26865
TITLE: Cannabimimetic arachidonylethanolamide (anandamide) derivatives as useful medications, and preparation thereof
INVENTOR(S): Makriyannis, Alexandros; Khanolkar, Atmaram; Goutopoulos, Andreas
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000032200	A1	20000608	WO 1999-US28136	19991124
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1049474	A1	20001108	EP 1999-961838	19991124
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRIORITY APPLN. INFO.:			US 1998-109615P	P 19981124
			WO 1999-US28136	W 19991124

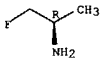
OTHER SOURCE(S): MARPAT 133:26865

IT **273734-17-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction; cannabimimetic arachidonylethanolamide derivative preparation for useful medication)

RN 273734-17-1 CAPLUS
CN 2-Propanamine, 1-fluoro-, hydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L4 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● HCl

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AB The fluorine chemical shifts (δF) of PhCHFCONHCHR1CH(Z)R2 (R1 = H, Me, CO2Me; R2 = Ph, Me; Z = OH, F) have been studied. The absolute configuration of R1CH(NH2)CHFR2 may be deduced from a comparison of the δF values of hydroxy amides of known configuration with the δF values of analogous fluoro amides.

ACCESSION NUMBER: 1993:559575 CAPLUS
DOCUMENT NUMBER: 119:159575
TITLE: 2-Fluoro-2-phenylacetic acid. Part 5. Fluorine NMR spectra of its amides prepared from hydroxy amines and fluoro amines
AUTHOR(S): Hamman, S.
CORPORATE SOURCE: UFR Chim., Univ. Joseph Fourier, Grenoble, 38041, Fr.
SOURCE: Journal of Fluorine Chemistry (1993), 62(1), 5-13
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: French

IT **149884-81-1 149884-82-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of fluorophenylacetic acid)

RN 149884-81-1 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, hydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 149884-82-2 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, hydrochloride, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

L4 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AB Title compds. RCH2CH(R''NH)CXYCOR2 (I; R = H, H2NCHMe; R2 = HO, alkoxy, aryloxy, amino acid residue bonded by amino N; R'' = H, amino acid residue bonded at the carboxy C; at least one of R and R'' being other than H; X = halo; Y = H, halo) and a salt thereof, useful for treating gingivitis or periodontal disease (no data), are prepared L-Threonine in DMF was treated with PhCH2Br to give N,N-dibenzylthreonine benzyl ester which was converted in 4 steps to I (R = R'' = Y = H; R2 = HO2CCH2NH, X = F) (II). A tablet composition comprising II and an analog is given. Dental formulations are also given.

ACCESSION NUMBER: 1992:255187 CAPLUS
DOCUMENT NUMBER: 116:255187
TITLE: Preparation of halogenated aminohexanoates and aminobutyrates antimicrobial agents
INVENTOR(S): Seibel, William L.; Gardner, Joseph H.
PATENT ASSIGNEE(S): Procter and Gamble Co., USA
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

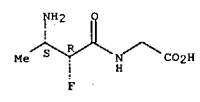
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5096700	A	19920317	US 1990-590427	19900928
PRIORITY APPLN. INFO.:			US 1990-590427	19900928

OTHER SOURCE(S): MARPAT 116:255187

IT **141483-43-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antimicrobial agent)

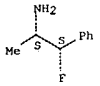
RN 141483-43-4 CAPLUS
CN Glycine, N-(3-amino-2-fluoro-1-oxobutyl)-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



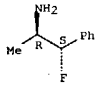
L4 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AB 1H and 19F NMR data for PhCHFCH2NRR1 (NRR1 = NH2, NH3+, NC5H10, NH+C5H10) and PhCHFCHRNR1R2 (I; R = Me, Ph; NR1R2 = NH2, NH3+, NC5H10, NH+C5H10, NHMe, NH2+Me, NMe2, NH+Me2) and those of the corresponding β-hydroxy-β-phenylamines were measured in CDCl3 and CD3OD. The predominant conformation for the protonated amines is that in which the ammonium group is antiperiplanar to the Ph group. Configurations (erythro and threo) for I were assigned based on coupling consts.
ACCESSION NUMBER: 1989:406795 CAPLUS
DOCUMENT NUMBER: 111:6795
TITLE: Configurational assignment of β-fluoro-β-phenylamines using -proton and fluorine-19 NMR
AUTHOR(S): Hamman, Sylvain; Benaissa, Tahar; Beguin, Claude G.
CORPORATE SOURCE: Lab. Cinet. Dyn. Mol., Univ. Grenoble I, St Martin d'Heres, 38402, Fr.
SOURCE: Magnetic Resonance in Chemistry (1988), 26(7), 621-4
CODEN: MRCHEG; ISSN: 0749-1581
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **74275-07-3 75197-98-7 75198-10-6 120978-82-7**
RL: PRP (Properties)
(NMR of)
RN 74275-07-3 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 75197-98-7 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 75198-10-6 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, hydrochloride, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

● HCl

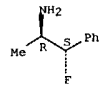
RN 120978-82-7 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, hydrochloride, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

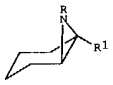
● HCl

L4 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AB Three methods were tested for the chemoselective title reaction: catalytic hydrogenation, catalytic transfer hydrogenation, and reduction with Ph3P. The last was the best.
ACCESSION NUMBER: 1988:422584 CAPLUS
DOCUMENT NUMBER: 109:22584
TITLE: Selective reduction of β-fluoro azides to β-fluoro amines
AUTHOR(S): Hamman, S.; Beguin, C. G.
CORPORATE SOURCE: Lab. Cinet. Dyn. Mol., Univ. Grenoble, St. Martin d'Heres, 38402, Fr.
SOURCE: Journal of Fluorine Chemistry (1987), 37(2), 191-6
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:22584
IT **75197-98-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 75197-98-7 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
GI



I

AB Ring-opening of secondary aziridines with anhydrous HF or Olah's reagent, and of N-activated aziridines by NEt3-nHF (n = 2, 2.5, 3) provides an efficient synthetic route to α,β-fluoroamines. The stereochem. of the reaction appears to be very dependent on the structure of the aziridine and on the fluorinating reagent. Thus in acyclic series, secondary aziridines can react with anhydrous HF with inversion of configuration, whereas Olah's reagent always leads to a carbocation formation which is then quenched by a fluoride ion delivered by the ammonium group. With bicyclic aziridines I (R = H, R1 = Ph, Et, H) this latter reaction yields cis-fluoroamines. In contrast, when N-carbo-tert-butoxy aziridines are treated with partially neutralized Olah's reagent (NEt3-nHF) exclusive inversion of configuration is observed in acyclic or cyclic series, leading from compds. I (R = CO2CMe3, R1 = Ph, Et, H) only to trans-fluoroamines. It is thus possible by proper choice of the fluorination method to direct the stereochem. of the final fluoroamine.
ACCESSION NUMBER: 1981:603644 CAPLUS
DOCUMENT NUMBER: 95:203644
TITLE: Ring opening of aziridines by different fluorinating reagents: three synthetic routes to α,β-fluoro amines with different stereochemical pathways
AUTHOR(S): Alvernhe, Gerard M.; Ennakoua, Christine M.; Lacombe, Sylvie M.; Laurent, Andre J.
CORPORATE SOURCE: Lab. Chim. Org. III, Univ. Claude Bernard, Villeurbanne, 69622, Fr.
SOURCE: Journal of Organic Chemistry (1981), 46(24), 4938-48
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:203644
IT **74275-07-3P 75197-98-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 74275-07-3 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 75197-98-7 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AB HF combines regiospecifically with aziridines to give 2-fluoro amines in good yields. F attack is in all cases completely directed to the most substituted ring carbon or to the benzylic carbon. The results are consistent with an SN1-type mechanism which involves isomerization of the pos. charged intermediate.
ACCESSION NUMBER: 1980:639100 CAPLUS
DOCUMENT NUMBER: 93:239100
TITLE: Preparation of fluoro amines by the reaction of aziridines with hydrogen fluoride in pyridine solution
AUTHOR(S): Wade, Tamsir N.
CORPORATE SOURCE: Lab. Chim. Struct. Org., Univ. Nice, Nice, 06034, Fr.
SOURCE: Journal of Organic Chemistry (1980), 45(26), 5328-33
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 93:239100
IT **74275-07-3P 75197-98-7P 75198-10-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 74275-07-3 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

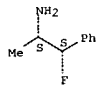
RN 75197-98-7 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 75198-10-6 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, hydrochloride, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



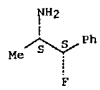
● HCl

L4 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
GI

I

AB Ring cleavage of aliphatic and aromatic aziridines by addition of Olah's reagent (HF, pyridine) was studied. Yields and regioselectivity are improved when using the corresponding N-activated aziridine and the less acidic fluorination reagent obtained by addition of Et3N to Olah's reagent. Thus, ring cleavage of the aziridine I (R = H) with HF-pyridine in C6H6 (20 h, 70°) gave, after benzoylation, 35% FCH2CH(NHBz)Me, and 65% MeCHFCH2NHBz (II) whereas similar treatment of I (R = Bz), omitting the benzoylation and in the presence of Et3N, gave 85% II.
ACCESSION NUMBER: 1980:445865 CAPLUS
DOCUMENT NUMBER: 93:45865
TITLE: Synthesis of α,β-fluoro amines from aziridines: position of ring opening and improvement of the fluorinating power of Olah's reagent
AUTHOR(S): Alvernhe, Gerard; Lacombe, Sylvie; Laurent, Andre
CORPORATE SOURCE: Lab. Chim. Org. III, Univ. Claude Bernard, Villeurbanne, F-69622, Fr.
SOURCE: Tetrahedron Letters (1980), 21(3), 289-92
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 93:45865
IT **74275-07-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 74275-07-3 CAPLUS
CN Benzeneethanamine, β-fluoro-α-methyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AB The apparent pK of 16 RCHFCHR1NR2R3 [R = H, Me, Et, Bu, Ph; R1 = H, Me (threo and erythro), Et; R2, R3 = H or alkyl] were determined by potentiometric titration in MeOCH2CH2OH-H2O. Substituent effects were discussed, e.g., the α-F decreases the basicity of the amine.

ACCESSION NUMBER: 1978:405760 CAPLUS
DOCUMENT NUMBER: 89:5760
TITLE: Determination of the dissociation constants of an α-fluorinated amines series in a water/2-methoxyethanol mixture
AUTHOR(S): Abdelkafi, Mohamed Mouldi; Baklouti, Ahmed
CORPORATE SOURCE: Lab. Chim. Org. Struct., Fac. Sci. Tunis, Tunis, Tunisia
SOURCE: Bulletin de la Societe Chimique de France (1977), (11-12, Pt. 1), 1044-8
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French

IT **66679-43-4 66679-44-5**
RL: PRP (Properties)
(dissociation constant of, in methoxyethanol-water)

RN 66679-43-4 CAPLUS
CN 2-Butanamine, 3-fluoro-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 66679-44-5 CAPLUS
CN 2-Butanamine, 3-fluoro-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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